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Development of a Theoretical Approach to Estimating the Water Permeability of Reverse Osmosis Membrane Materials

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Summary

To improve the antifouling properties of reverse osmosis membranes in seawater desalination processes, it is essential to elucidate the fouling phenomena at the atomistic level. In this study, we evaluated the microscopic interactions between betaine materials which have excellent antifouling properties and organic foulants, by using molecular dynamics (MD) simulations. Nonpolar *n*-undecane molecule was used as a model organic foulant. Simulation cells of betaine/n-undecane binary mixtures were constructed and the content of n-undecane molecules was set to approximately 50 wt%. For the equilibrated binary mixture systems, MD simulations were conducted to evaluate the microscopic interactions between betaine moieties and *n*-undecane molecules. Here, second virial coefficients were calculated to assess the aggregation/dispersion properties of the binary mixture systems. Mean square displacements (MSDs) were also calculated to estimate the molecular mobilities of betaine moieties and *n*-undecane molecules.

The elapsed time dependences of the MSDs indicated that the accuracies of statistical samplings become dramatically higher with an increase in temperature. In addition, the types of betaine moieties which are less compatible with n-undecane molecules have higher molecular mobilities in the binary mixtures. We had expected that the molecular mobilities of betaine moieties would become lower when they agglomerate, because the robust ionic interactions between the anionic group and the cationic group are dominant. Intriguingly, the opposite trend to this expectation was observed in our simulations. Although the effects of the difference in the molecular weights of betaine moieties should be considered in the future, the qualitative agreement between the order of aggregation/dispersion properties and that of molecular mobilities certainly indicates the correlation between the two criteria.

Furthermore, the type of betaine moiety which exhibited the most excellent antifouling property was similar to the type of betaine moiety which was indicated in a previous study. The optimization of the modeling and the simulation conditions in MD simulations are certainly promising to elucidate membrane fouling phenomena.